Flux Calculations in the Heat Transfer Component of TELLURIDE

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The TELLURIDE project at Los Alamos is a strategic computing effort aimed at producing high fidelity simulations of metal solidification processes. Its code provides numerical simulations of solidification, fluid flow, heat transfer, phase transformations, mechanical deformation, and welding processes on the kinds of meshes seen in Fig. 1. The simulation of each component is driven by a discretization of the continuum equations describing the physical processes. The components are then coupled in a way that describes their true physical interaction.

The ability of projects like TELLURIDE to model physical reality depends on several factors: accurate numerical models, stable computer implementations, realistic test data, and fast parallel algorithms. So when the simulations are unable to approximate reality, it can be quite difficult to find where things went awry. However, prior to executing any simulation, one can perform component testing, whereby ensuring that each component accurately models the physics it is supposed to describe. Here, we investigate inaccuracies in the heat transfer component that are due to a poor approximation of the heat flux using existing methodologies. Furthermore, we describe a robust approximation scheme for calculating the heat flux that is based on the support-operators (SO) methodology [1].

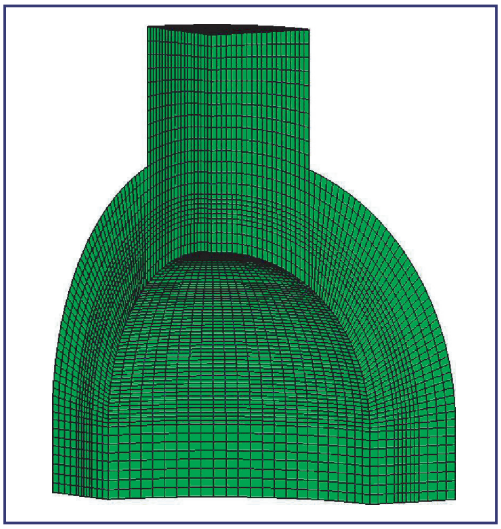

Figure 1— Typical TELLURIDE mesh.

The flux calculations within the heat transfer component arise within the nonlinear equation that describes the temporal change of specific enthalpy. The equation is discretized using finite volumes on a hexahedral mesh, and then flux values are computed on cell faces given cell-centered temperature values. There are two approaches to computing the flux. Both obtain the flux by combining a gradient calculation with knowledge of the conductivity and the normal vector. Where they differ is how the gradient is computed. Approach **A** computes the gradient on each face via the definition of the directional derivative. This yields a gradient that depends on the difference of the temperature values at the two adjacent cells and the vector directed from one cell center to the other. Approach **B** is a much more sophisticated algorithm that depends on surrounding cells. See [2] for a detailed description. The limitations of the two approaches are that approach **A** is inaccurate for nonorthogonal meshes, while approach **B** is inaccurate when there are jumps in the conductivity.

We observe the two approaches' limitations for a simple problem on the unit cube. Specifically, for a smooth meshing of the unit cube (Fig. 2), a conductivity and a temperature distribution are defined. Then the normal component of the flux is calculated for each face and its deviation from the true value is measured. We use a conductivity of $\kappa = 1$ for $x \le 1/2$ and $\kappa = 100$ for $x > 1/2$, and a temperature distribution given by

$$T(x,y,z) = \begin{cases} x, & \text{for } x \le 1/2 \\ \dfrac{1}{200}(2x+99), & \text{for } x > 1/2 \end{cases}.$$

For a sequence of smooth grids like in Fig. 2, we illustrate with the blue lines in Fig. 3 the lack of convergence of the interior and boundary root mean-squared error for approach **A**. We see the same type of divergence for approach **B**.

The SO approach relies on the SO discretization for diffusion-type equations. Similar to the approach **B** method, the computed flux depends on more than just the two adjacent cell-centered temperature values. However, in contrast to approach **B**, the SO approach correctly incorporates conductivity information so that inaccuracies do not arise from discontinuous conductivities. Again, see [1] for further details.

In the heat transfer we use SO in the following way. To begin, we explicitly compute a flux rather than taking an intermediate step of computing a gradient. However, like approach **A**, we do compute a vector for each face of each cell that depends on the difference of the temperature between the two adjacent cells. We then employ this vector as the right-hand side of the appropriate matrix problem, i.e., a system of the form $Au = f$. Finally, we must solve this large system of algebraic equations using an iterative solution method. That is, we find the solution, say u, by making an initial guess and then iteratively improving it until we have the accuracy that we desire. For the same problem for which approach **A** showed no convergence, we get convergence for the SO approach. This is seen in red in Fig. 3.

The SO approach to heat flux calculations offers a drastic improvement to the current approaches when the mesh is severely distorted or the conductivity jumps across material interfaces. The approach however is more costly. Yet, because all other approaches suffer from their inaccuracies for more difficult problems, the cost of the SO approach is an adequate price to pay. Moreover, in the future, we will be investigating the accuracy of more efficient local solution methods.

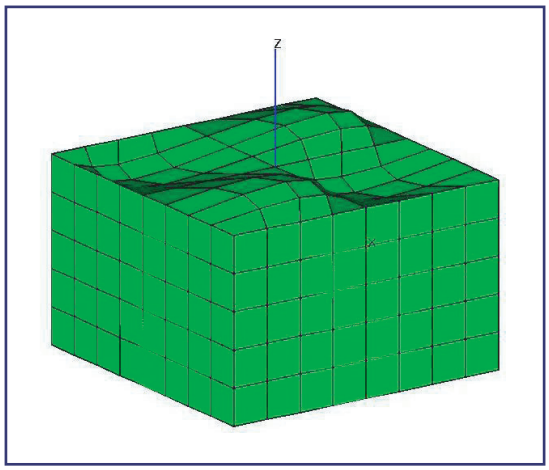

Figure 2—
Slice of smooth 3D mesh.

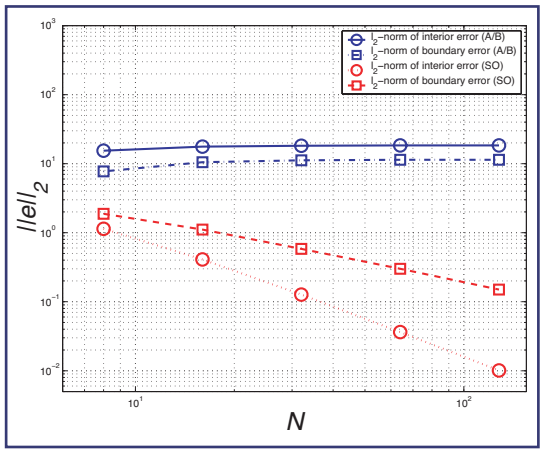

Figure 3—
Illustration of lack of convergence for existing approach (A/B), and illustration of convergence for support-operators (SO) on a sequence of finer grids.

[1] J. Hyman, et al., "Mimetic Finite Differences for Diffusion Equations," *Comput. Geosc.* **6**, pp. 333–352, 2002.
[2] T.J. Barth, "Aspects of Unstructured Grids and Finite-Volume Solvers for Euler and Navier-Stokes Equations," *KI/NASA/AGARD Special Course on Unstructured Grid Methods for Advection Dominated Flows* (AGARD Publication R-787), 1995.

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